

Sunday 21/9

14.00-19.00

Welcome to Girona

20.00-23.30

Informal dinner

Monday 22/9

09.00

Leaving hotel for venue first day (Facultat de Medicina, UdG)

09.15-09.30

Registration (Sala d'Actes, Fac. Medicina)

09.30-09.45

Opening Workshop (Vice-rector of Economy and Infrastructures UdG)

09.45-10.15

General Introduction (M. Swart)

10.15-11.15

Session I: Let's Get to Know Each Other

11.15-11.20

Group picture

11.15-11.45

Coffee break

11.45-13.30

Session II: Let's Get to Know Each Other

13.30-14.30

Lunch break

14.30-16.00

Session III: Let's Get to Know Each Other

16.00-16.30

Coffee break

16.30-18.00

Session IV: Let's Get to Know Each Other

18.00-19.00

Pica-pica

19.00-20.00

Back to hotel

20.30-23.30

Conference dinner (Restaurant Casa Marieta)

Tuesday 23/9

09.00

Leaving hotel for venue second day (Facultat de Ciències, UdG)

09.30-10.15

WG1: PB2

(M. Gruden-Pavlovic, M. Swart)

10.15-10.35

WG2: Sala de Graus

WG3: PB2

WG4: PB6

Aims and scope

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(M. Stein)

(R. Deeth)

(K. Ray)

10.35-10.55

Borowski

Morgan

Sanakis

10.55-11.15

Carvalho

Balazs

Orio

11.15-11.45

Coffee break

11.45-12.05

Escudero

Müller

Codolà

12.05-12.25

Feixas

Enachescu

Krewald

12.25-12.45

Radon

Weber

Paraskevopoulou

12.45-13.05

Simaan

Zlatar

de Visser

13.05-13.30

Discussion

Discussion

Discussion

13.30-14.30

Lunch break

14.30-17.30

Management Committee Meeting: Sala de Graus

14.30-17.30

(working area available for non-MC members in PB2/PB6)

19.00-20.30

Guided tour through city center Girona

21.00-23.30

Informal dinner

Wednesday 24/9

All day

Travel back home

Seminars Tuesday 23-9

<i>Presenter</i>	<i>Title</i>
Pinter Balazs	Dependence of DFT spin-state energetics on exact exchange for representative transition metal complexes
Tomasz Borowski	Spin states and reaction mechanisms of mononuclear non-heme metalloenzymes - computational studies
Alexandra Carvalho	Computational studies of metalloproteins
Zoel Codolà	Molecular iron complexes for water oxidation catalysis
Christian Enachescu	Elastic models in spin crossover compounds
Daniel Escudero	DFT/MRCI studies on transition metal complexes
Ferran Feixas	A Molecular Dynamics Investigation of Mycobacterium tuberculosis Prenyl Synthases: Conformational Flexibility, Biomolecular Recognition and Implications for Computer-Aided Drug Discovery
Vera Krewald	Magnetic interactions in nature's water splitting complex and synthetic analogues
Grace Morgan	Ordering Phenomena in Spin Crossover Solids
Danny Müller	Fe(II) Spin Crossover with N1-substituted tetrazoles
Maylis Orio	Theoretical investigation of a Cu(II)-phenoxyl radical complex formed at a low negative potential
Patrina Paraskevopoulou	Developing New Catalytic Systems for Radical and Metathesis Polymerization Reactions
Mariusz Radon	Spin States of Heme-Related Models: Accurate Energetics from Coupled Cluster Calculations and Role of Spin States in Ligand Binding
Ioannis Sanakis	The electronic states of natural and synthetic multinuclear transition metal clusters probed by spectroscopic techniques
Jalila Simaan	Investigation of a non-heme iron(II) containing enzyme: ACC Oxidase
Sam de Visser	There is no such thing as an iron(V)-oxo!
Birgit Weber	Spin Crossover Complexes with Schiff base-like Ligands
Matija Zlatař	Application of Density Functional Based Ligand Field Theory to Spin States